Biochar-Catalyzed Synthesis of Functionalized Heterocycles: Design, Development and Evaluation of Sustainable Catalytic Protocols

SYNOPSIS

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SYNOPSIS OF RESEARCH WORK FOR Ph.D. DEGREE IN THE FACULTY OF SCIENCE (CHEMISTRY)

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(i) Work Plan

a. Purpose and need of the study

The development of environmentally benign and economically viable catalytic systems has become a major priority in contemporary synthetic organic chemistry. Traditional homogeneous and heterogeneous catalysts often suffer from drawbacks such as high cost, toxicity, poor recyclability, and energy-intensive preparation. These limitations create an urgent need for greener alternatives that align with the principles of sustainable chemistry. Biochar, an inexpensive, carbon-rich material produced through the pyrolysis of biomass, has emerged as a promising catalyst and catalyst support due to its abundant surface functionalities, high thermal stability, tunable porosity, and potential for chemical modification. Its production from agricultural waste, forestry residues, and animal-derived biomaterials further strengthens its suitability as a renewable, circular-economy-based catalytic material. Heterocyclic compounds occupy a central position in pharmaceuticals, agrochemicals, natural products, and functional materials. Yet, many conventional methods for their synthesis rely on harsh conditions, hazardous reagents, or non-recyclable catalysts. Biochar-based catalytic systems present a sustainable alternative capable of supporting acid–base functionalities, metal anchoring, and ionic or magnetic modifications, enabling efficient transformations under mild and eco-friendly reaction conditions. This study aims to systematically develop, optimize, and evaluate biochar-derived catalytic systems for the synthesis of functionalized heterocycles of pharmacological and industrial relevance. The use of biochar not only minimizes environmental impact but also improves catalyst lifetime and reduces process cost. The work seeks to bridge the existing gap in applying biochar to heterocyclic synthesis by establishing robust, recyclable, and high-performance catalytic

methodologies, thereby contributing to the growing field of sustainable chemistry.

Review of Literature of proposed work

Recent years have witnessed a surge in research on biochar-based catalysts due to their sustainability, ease of preparation, and adaptability for structural modification. Studies have demonstrated that biochar derived from diverse biomass sources, such as agricultural residues, chicken manure, wood chips, and plant waste, can be engineered to incorporate acidic groups, metal nanoparticles, ionic species, or magnetic components, significantly enhancing catalytic efficiency. Biochar-supported catalysts have shown promising performance in various transformations, including oxidations, reductions, condensations, esterifications, and multi-component reactions. Several reports highlight the potential of functionalized biochar in promoting heterocyclic syntheses such as chromenes, pyrans, tetrazoles, quinazolinones, and pyrazole derivatives. The immobilization of transition metals like Cu, Ni, Fe, and rare-earth elements on biochar matrices has further expanded its catalytic scope. Despite these advances, literature reveals limited systematic studies on integrating biochar catalysts specifically for the synthesis of structurally diverse and highly functionalized heterocycles. Additionally, mechanistic insights, structure, activity relationships, and comparative performance analyses remain underexplored. Therefore, existing research underscores the feasibility of biochar as a sustainable catalyst while also emphasizing the need for comprehensive studies focused on heterocycle-oriented applications. This project aims to address these gaps by developing optimized catalytic systems for targeted heterocyclic frameworks.

b. Details of the project with chapterization

Chapter- I: Introduction

Chapter- II: Survey of previous works

Chapter- III : Experimental

Chapter- IV: Result and Discussion

Chapter- V : Conclusion

Chapter I: Introduction

This chapter will provide an overview of sustainable catalysis with emphasis on the growing relevance of biochar as an eco-friendly catalytic material. It will outline the limitations of conventional catalysts and introduce the structural features, surface chemistry, and tunability of biochar that make it suitable for green synthesis. The fundamental importance of heterocyclic compounds in pharmaceuticals, agrochemicals, and materials science will also be highlighted. Overall, the chapter will establish the rationale for exploring biochar-assisted methodologies for the sustainable synthesis of functionalized heterocycles.

Chapter II: Survey of Previous Works

This chapter will summarize major advancements in biochar production, modification strategies, and catalytic applications. Literature on acid-treated, metal-doped, ionic-liquid-functionalized, and magnetic biochar catalysts will be critically reviewed. Previous studies involving multicomponent reactions, carbon–carbon bond-forming processes, and heterocycle construction will be discussed. Existing gaps, such as limited substrate scope, inadequate mechanistic insights, and insufficient catalyst recyclability, will be highlighted to justify the need for the proposed research.

Chapter III: Experimental

This chapter will outline the proposed experimental plan, including the preparation of biochar from selected biomass sources and its subsequent functionalization through acid treatment, metal incorporation, or magnetic modification. Planned characterization techniques such as FTIR, PXRD, SEM, BET, TGA, and VSM will be described. The proposed synthetic procedures for generating heterocycles using biochar catalysts will be presented, along with strategies for reaction optimization, catalyst-loading studies, and recyclability assessments.

Chapter IV: Results and Discussion

This chapter will later present and interpret the experimental findings, including catalytic activity, reaction efficiencies, and substrate scope. Expected discussions will cover mechanistic pathways, structure, activity relationships, and the influence of biochar functionalization on catalytic performance. Catalyst stability, recyclability, and comparative evaluation with traditional catalysts will also be included. Spectral and graphical data will support the analytical interpretations.

Chapter V: Conclusion

This chapter will summarize the anticipated outcomes of the study, emphasizing the potential of biochar-derived catalysts to offer a sustainable, efficient, and cost-effective platform for heterocycle synthesis. The advantages of green reaction conditions, improved catalytic performance, and catalyst reusability will be highlighted. The chapter will also outline possible limitations and future research directions, such as enhancing catalyst design, expanding substrate diversity, and exploring broader applications in organic synthesis.

c. Hypothesis

It is hypothesized that biochar catalyzed reactions will provide an efficient, environmentally friendly, and high-yielding synthetic route to structurally diverse substituted heterocycles. By carefully optimizing reaction parameters, such as catalyst type, solvent, temperature, and reagent ratios, it is expected that a wide range of heterocycles can be generated with improved purity and selectivity. Due to the established biological relevance of heterocycle frameworks, the newly synthesized derivatives are anticipated to exhibit promising biological activities. Furthermore, the use of a unified multicomponent strategy is expected to enhance molecular diversity while minimizing reaction steps, waste generation, and overall environmental impact.

D. Methodology

The proposed research will involve the development and evaluation of biochar-based catalytic systems for the synthesis of functionalized heterocyclic compounds. Initially,

suitable biomass sources (such as agricultural or plant waste) will be selected and subjected to controlled pyrolysis to produce biochar. The pyrolysis parameters, including temperature, heating rate, and atmospheric conditions, will be optimized to obtain biochar with the desired porosity and surface functionality. In the next stage, the biochar will be chemically modified to introduce catalytic activity. Functionalization methods may include acid treatment, metal loading, or magnetic modification, depending on the intended application. These procedures will be planned using established protocols from the literature, and the feasibility will be evaluated during the experimental phase. The prepared biochar samples will then be characterized using techniques such as FTIR, PXRD, SEM, BET surface area analysis, TGA, and VSM (for magnetic materials). These characterizations will help determine the structural and surface properties required for catalytic performance. Following catalyst preparation, we propose to apply the optimized biochar systems to the synthesis of variety of heterocycles, using step-wise or multicomponent reactions. Reaction conditions (solvent, temperature, catalyst loading, and time) will be optimized during the experimental stage. Recyclability and reusability tests will also be planned to evaluate catalyst stability under repeated use. Mechanistic pathways will be proposed based on preliminary observations, literature reports, and reaction outcomes obtained during the course of the study. Green chemistry parameters such as atom economy and waste reduction will be evaluated to assess sustainability.

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